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SOME NEW ALGORITHMS FOR BOUNDARY VALUE PROBLEMS IN SMOOTH PARTICLE HYDRODYNAMICS

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A rederivation of the basic equations of smoothed particle hydrodynamics is given that removes some of the intuitive elements in earlier work. New algorithms are obtained for hydrodynamics with heat flow that include boundary terms. These algorithms permit application of the method to systems driven by external pressures or heat sources. Hydrodynamic work terms are different in the new algorithms and these terms may eliminate some difficulties encountered with expressions found in the literature. The method developed for thermal diffusion yields the fluxes directly and may be extended to a flux-limited diffusion formulation of radiation transport. (Keywords.)

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PREFACE

The author thanks Robert F. Stellingwerf for introducing him to the SPH method and for many enlightening discussions. This work was supported under Contract DNA 001-88-C-0079.

CONVERSION TABLE

Conversion factors for U.S. Customary to metric (SI) units of measurement

MULTIPLY → / ← TO GET	BY → / ← BY	TO GET / DIVIDE
angstrom	1.000 000 X E -10	meters (m)
atmosphere (normal)	1.013 25 X E +2	kilo pascal (kPa)
bar	1.000 000 X E +2	kilo pascal (kPa)
barn	1.000 000 X E -28	meter^2 (m^2)
British thermal unit (thermochemical)	1.054 350 X E +3	joule (J)
calorie (thermochemical)	4.184 000	joule (J)
cal (thermochemical)/cm^2	4.184 000 X E -2	mega joule/m^2 (MJ/m^2)
curie	3.700 000 X E +1	*giga becquerel (GBq)
degree (angle)	1.745 329 X E -2	radian (rad)
degree Fahrenheit	$t_K = (t°f + 459.67)/1.8$	degree kelvin (K)
electron volt	1.602 19 X E -19	joule (J)
erg	1.000 000 X E -7	joule (J)
erg/second	1.000 000 X E -7	watt (W)
foot	3.048 000 X E -1	meter (m)
foot-pound-force	1.355 818	joule (J)
gallon (U.S. liquid)	3.785 412 X E -3	meter^3 (m^3)
inch	2.540 000 X E -2	meter (m)
jerk	1.000 000 X E +9	joule (J)
joule/kilogram (J/kg) (radiation dose absorbed)	1.000 000	Gray (Gy)
kilotons	4.183	terajoules
kip (1000 lbf)	4.448 222 X E +3	newton (N)
kip/inch^2 (ksi)	6.894 757 X E +3	kilo pascal (kPa)
ktap	1.000 000 X E +2	newton-second/m^2 (N-s/m^2)
micron	1.000 000 X E -6	meter (m)
mil	2.540 000 X E -5	meter (m)
mile (international)	1.609 344 X E +3	meter (m)
ounce	2.834 952 X E -2	kilogram (kg)
pound-force (lbs avoirdupois)	4.448 222	newton (N)
pound-force inch	1.129 848 X E -1	newton-meter (N·m)
pound-force/inch	1.751 268 X E +2	newton/meter (N/m)
pound-force/foot^2	4.788 026 X E -2	kilo pascal (kPa)
pound-force/inch^2 (psi)	6.894 757	kilo pascal (kPa)
pound-mass (lbm avoirdupois)	4.535 924 X E -1	kilogram (kg)
pound-mass-foot^2 (moment of inertia)	4.214 011 X E -2	kilogram-meter^2 (kg·m^2)
pound-mass/foot^3	1.601 846 X E +1	kilogram/meter^3 (kg/m^3)
rad (radiation dose absorbed)	1.000 000 X E -2	**Gray (Gy)
roentgen	2.579 760 X E -4	coulomb/kilogram (C/kg)
shake	1.000 000 X E -8	second (s)
slug	1.459 390 X E +1	kilogram (kg)
torr (mm Hg, 0° C)	1.333 22 X E -1	kilo pascal (kPa)

*The becquerel (Bq) is the SI unit of radioactivity; 1 Bq = 1 event/s.
**The Gray (Gy) is the SI unit of absorbed radiation.

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SECTION 1

INTRODUCTION

Although particle methods in hydrodynamics have been remarkably successful in many problems,[1-4] current methods suffer from an inadequate treatment of boundary conditions. This is particularly evident when one tries to include heat transport in the energy equation.[5-6] Without accurate values of the flux at the boundaries, it is not possible to calculate the net exchange of energy between a fluid and its environment.

Another class of problems requiring accurate treatment of boundary conditions is illustrated by the shock tube problem where the shock is driven by a piston.

In this case the particle method must be able to accommodate an externally-applied (boundary) pressure. The method should also be able to handle conduction heating of the gas by a hot wall or piston; and, finally, boundaries must be treated accurately to include radiative heat exchange, in particular, radiative cooling.

In this paper, some new algorithms are developed for smooth particle hydrodynamics in problems where external boundary conditions are imposed. Although thermal and radiative diffusion are included, radiation transport is neglected in the present paper.

SECTION 2

KERNEL ESTIMATES NEAR BOUNDARIES

The standard kernel estimate of a function is given by[3]

$$f_\kappa(x) = \int_o^X f(x')W(x - x', h)dx' , \tag{1}$$

where the kernel is normalized by

$$\lim_{h \to o} \int_o^X W(x - x', h)dx' = 1 . \tag{2}$$

In these expressions the domain of definition is $0 \leq x \leq X$.

As long as $h \to 0$ one would not expect normalization problems near the boundary, but in practical applications kernels with finite h are used. One would then expect difficulties within $x \sim h$ of the boundary because the integrals are truncated by the boundary. For example

$$\lim_{x \to X} \int_o^X W(x - x')dx' = \frac{1}{2} , \tag{3}$$

which is obvious from Fig. 1.

Consider what this does to the kernel estimate of the density. Assume a dense constant spacing of particles in the vicinity of the boundary X. Far from the wall, the kernel estimate gives

$$\begin{aligned} \rho(x) &= \int_o^X \rho(x')W(x - x', h)dx' \\ &\simeq m \sum_j W(x - x_j, h) \\ &= \rho_c , \end{aligned} \tag{4}$$

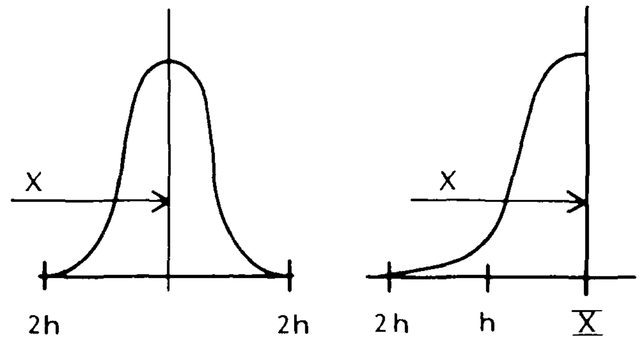

Figure 1. A typical smoothing kernel, showing how the symmetrical form is truncated as the particle approaches a boundary.

where ρ_c is the constant value. However, following Eq. 3, as $x \to X$, the kernel estimate becomes

$$\begin{aligned} \rho(X) &= \lim_{x \to X} \int_o^X \rho(x') W(x - x', h) dx' \\ &= m \sum_j W(X - x_j, h) \\ &= \frac{1}{2} \rho_c \, . \end{aligned} \tag{5}$$

So within $\sim h$ of the boundary the interpolation feature of the kernel estimate gives spurious results. Also, presumably, one finds

$$\begin{aligned} P(X) &= \lim_{x \to X} \int_o^X P(x') W (x - x') dx' \\ &= \frac{1}{2} P_c \, , \end{aligned} \tag{6}$$

for the case of a uniform pressure in the neighborhood of the boundary as in Fig. 2.

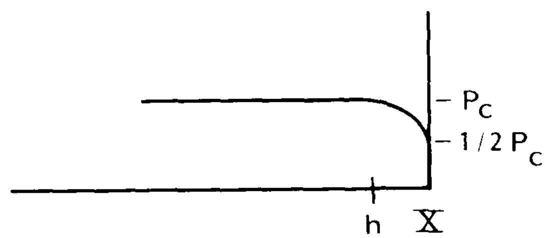

Figure 2. The falloff in a uniform pressure distribution as given by a kernel estimate in the neighborhood of the boundary.

In summary, we have seen that because of the truncation of the normalization integral within $\sim h$ of a boundary, interpolation implied by the kernel estimate may not be accurate. Renormalization is a possibility but does not appear to work. Also, the boundary value method presented below seems to require the apparent failure manifested in Eq. 3.

SECTION 3

MOMENTUM EQUATION WITH BOUNDARY PRESSURE

All treatments of SPH of which the author is aware require integration by parts when deriving kernel estimates but simply drop the boundary terms. (See Section 8 below.) This is presumably because the kernel is supposed to mimic a δ-function which goes to zero sufficiently far from the particles representing the edge of the system.

However, if we are to consider problems where the particles interact with a boundary condition, such as an externally-applied pressure, we must specifically include the boundary terms. In this section the two procedures developed by Monaghan for the momentum equation[2,3] are modified to include boundary pressure.

In the first case, write the momentum equation as

$$\begin{aligned} \frac{dv}{dt} &= -\frac{1}{\rho}\frac{\partial P}{\partial x} \\ &= -\frac{\partial}{\partial x}\left(\frac{P}{\rho}\right) - \frac{P}{\rho^2}\frac{\partial \rho}{\partial x}. \end{aligned} \tag{7}$$

The kernel estimate of this equation is formed by changing the independent variable to x', multiplying by $W(x-x')dx'$ and integrating over the domain $0 \le x \le X$. One obtains

$$\begin{aligned} \frac{dv_\kappa}{dt} &= -\int_o^X \frac{\partial}{\partial x'}\left(\frac{P}{\rho}\right) W(x-x')dx' \\ &\quad -\left(\frac{P}{\rho^2}\right)_\kappa \int_o^X \frac{\partial \rho}{\partial x'} W(x-x')dx' , \end{aligned} \tag{8}$$

where the subscript κ denotes "kernel estimate." The second integral has been linearized by evaluating (P/ρ^2) by its kernel estimate and taking it outside the integral sign. This is justified since $W(x-x')$ acts like $\delta(x-x')$.

After integrating by parts, one finds

$$\frac{dv_\kappa}{dt} = -\left[\frac{P}{\rho}W(x-x')\right]_o^X - \int_o^X \left(\frac{P}{\rho}\right)\frac{\partial W(x-x')}{\partial x}dx'$$
$$-\left(\frac{P}{\rho^2}\right)_\kappa [\rho W(x-x')]|_o^X - \left(\frac{P}{\rho^2}\right)_\kappa \int_o^X \rho\frac{\partial W(x-x')}{\partial x}dx' \,, \qquad (9)$$

where we have used $\partial W/\partial x = -\partial W/\partial x'$ assuming a symmetric kernel.

If we now evaluate the integrals by the particle method, replacing

$$\int f(x')W(x-x')dx' \rightarrow \sum_j f_j W(x-x_j)\frac{m_j}{\rho_j} \,, \qquad (10)$$

we obtain an expression for the momentum equation with external boundary pressures,

$$\frac{dv_i}{dt} = \left[\left(\frac{P}{\rho^2}\right)_o + \left(\frac{P}{\rho^2}\right)_i\right]\rho_o W(x_i - o)$$
$$-\left[\left(\frac{P}{\rho^2}\right)_X + \left(\frac{P}{\rho^2}\right)_i\right]\rho_X W(x_i - X)$$
$$-\sum_j m_j \left[\left(\frac{P}{\rho^2}\right)_j + \left(\frac{P}{\rho^2}\right)_i\right]\frac{\partial W(x_i - x_j)}{\partial x_i} \,. \qquad (11)$$

Thus, particle i feels the effect of the boundary pressure if it is within range of the boundary and $W(x_i - o) \neq 0$. The boundary pressure enters in a term similar to that for any other particle j.

Does this expression conserve momentum? If we multiply by m_i and sum, we find

$$
\begin{aligned}
\frac{d}{dt}\sum_i m_i v_i &= \rho_o \sum_i m_i \left[\left(\frac{P}{\rho^2}\right)_o + \left(\frac{P}{\rho^2}\right)_i\right] W(x_i - o) \\
&\quad - \rho_X \sum_i m_i \left[\left(\frac{P}{\rho^2}\right)_X + \left(\frac{P}{\rho^2}\right)_i\right] W(x_i - X) \\
&\quad - \sum_i \sum_j m_i m_j \left[\left(\frac{P}{\rho^2}\right)_j + \left(\frac{P}{\rho^2}\right)_i\right] \frac{\partial W(x_i - x_j)}{\partial x_i} \ .
\end{aligned}
\tag{12}
$$

The last term in the equation vanishes because $\partial W/\partial x_i$ is antisymmetric in i and j. To get a form where P_i and P_j appear symmetrically was the main point in the manipulation of P and ρ in Eq. 7. This insures the vanishing of the last term in Eq. 12 which is necessary for conservation.

Now what about the boundary terms? From Eq. 3, we have

$$
\sum_i m_i W(x_i - o) = \frac{1}{2}\rho_o \ , \tag{13}
$$

so that Eq. 12 becomes

$$
\begin{aligned}
\frac{d}{dt}\sum_i m_i v_i &= \frac{1}{2}P_o + \rho_o \sum_i m_i \left(\frac{P}{\rho^2}\right)_i W(x_i - o) \\
&\quad - \frac{1}{2}P_X - \rho_X \sum_i m_i \left(\frac{P}{\rho^2}\right)_i W(x_i - X) \ .
\end{aligned}
\tag{14}
$$

Here P_o and P_X are the given boundary values of the external pressure. The other terms are the interpolated values of the pressure at the boundary given by the internal calculation. If this calculation is accurate (apart from the factor of $1/2$), it must yield

$$
\frac{1}{2}P_o \simeq \rho_o \sum_i m_i \left(\frac{P}{\rho^2}\right)_i W(x_i - o) \ , \tag{15}
$$

and

$$\frac{1}{2}P_X \simeq \rho_X \sum_i m_i \left(\frac{P}{\rho^2}\right)_i W(x_i - X) \ , \tag{16}$$

giving for Eq. 12

$$\frac{d}{dt}\sum_i m_i v_i = P_o - P_X \ . \tag{17}$$

A similar analysis is possible for Monaghan's other conservative form of the momentum equation. First write

$$\frac{dv}{dt} = -\frac{1}{\rho}\frac{\partial P}{\partial x} = -2\frac{P^{1/2}}{\rho}\frac{\partial P^{1/2}}{\partial x} \ . \tag{18}$$

Then the kernel estimate of the momentum equation becomes

$$\begin{aligned} \frac{dv_k}{dt} &= -2\left(\frac{P^{1/2}}{\rho}\right)_\kappa \int_o^X \frac{\partial P^{1/2}}{\partial x'} W(x-x')dx' \\ &= -2\left(\frac{P^{1/2}}{\rho}\right)_\kappa P^{1/2}W\Big]_o^X \\ &\quad - 2\left(\frac{P^{1/2}}{\rho}\right)_\kappa \int_o^X P^{1/2}\frac{\partial W}{\partial x}(x-x')dx' \ . \end{aligned} \tag{19}$$

Evaluating the integral by the particle method gives

$$\begin{aligned} \frac{dv_i}{dt} &= 2\left(\frac{P^{1/2}}{\rho}\right)_i \left[P_o^{1/2}W(x_i - o) - P_X^{1/2}W(x_i - X)\right] \\ &\quad - 2\sum_j m_j \frac{P_i^{1/2}P_j^{1/2}}{\rho_i\rho_j}\frac{\partial W(x_i - x_j)}{\partial x_i} \ , \end{aligned} \tag{20}$$

where, again, we note the fortuitous appearance of the factor of 2 in the boundary terms which will compensate the falloff represented by Eq. 3.

After multiplying by m and summing, we obtain

$$\begin{aligned}\frac{d}{dt}\sum_i m_i v_i &= 2P_o^{1/2}\sum_i m_i \left(\frac{P^{1/2}}{\rho}\right)_i W(x_i - o) \\ &\quad - 2P_X^{1/2}\sum_i m_i \left(\frac{P^{1/2}}{\rho}\right)_i W(x_i - X) \\ &\quad - 2\sum_i\sum_j m_i m_j \frac{P_i^{1/2}P_j^{1/2}}{\rho_i\rho_j}\frac{\partial W(x_i - x_j)}{\partial x_i} \ ,\end{aligned} \tag{21}$$

where because of the symmetry in i and j, the last term is zero; and since

$$\begin{aligned}\frac{1}{2}P_o^{1/2} &\simeq \sum_i m_i \left(\frac{P^{1/2}}{\rho}\right)_i W(x_i - o) \ , \\ \frac{1}{2}P_X^{1/2} &\simeq \sum_i m_i \left(\frac{P^{1/2}}{\rho}\right)_i W(x_i - X) \ ,\end{aligned} \tag{22}$$

we get the conservation of momentum,

$$\frac{d}{dt}\sum_i m_i v_i = P_o - P_X \ . \tag{23}$$

It is curious that in both of these forms the boundary terms enter in such a way that the factor of 1/2 from the normalization anomaly at the boundary is required for a conservative momentum equation. This is not true of all forms, however. For example, the first expression for the pressure gradient in Eq. 7 does not produce a boundary term with the factor of 2 present.

SECTION 4

EQUIVALENT FINITE DIFFERENCE FORMS

If particles are assumed equally spaced, it is possible to derive the equivalent finite difference form which the kernel estimate represents.[6] It is instructive to look at these forms, particularly in the neighborhood of the boundary, to get a feeling for the accuracy of the particle method.

For the purpose of illustration, consider the kernel shown together with its derivative in Fig. 3,[2,6]

$$W(x-x') = \begin{cases} \dfrac{1}{h}\left(\dfrac{2}{3} - u^2 + \dfrac{1}{2}|u|^3\right) & 0 \le |u| \le 1 \\[2ex] \dfrac{1}{6h}(2-|u|)^3 & 1 \le |u| \le 2 \\[2ex] 0 & 2 \le |u| \, , \end{cases} \tag{24}$$

where $u = (x - x')/h$, and

$$\frac{\partial W}{\partial x} = \frac{1}{h}\frac{\partial W}{\partial u} \, . \tag{25}$$

Now, consider a series of equally spaced equal mass particles far from any boundary as shown in Fig. 4. The momentum equation in the form of Eq. 11 is

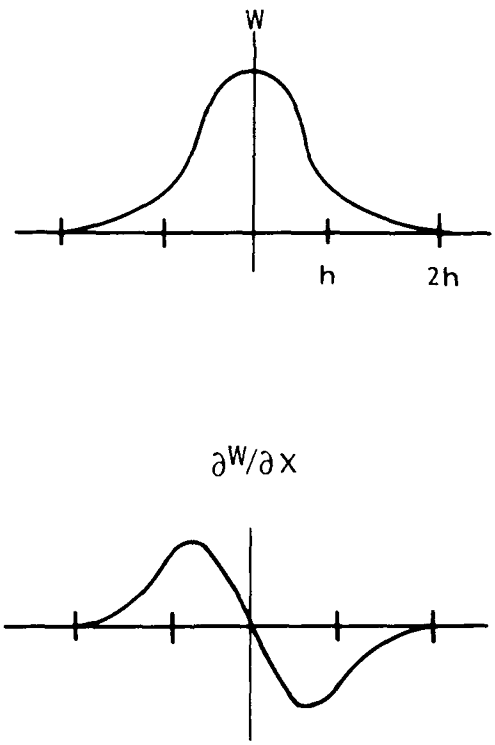

Figure 3. The smoothing kernel given by Eq. 24 and its (continuous) first derivative.

$$
\begin{aligned}
\frac{dv_i}{dt} &= -m\sum_j\left[\left(\frac{P}{\rho^2}\right)_j+\left(\frac{P}{\rho^2}\right)_i\right]\frac{\partial W(x_i-x_j)}{\partial x_i} \\
&= -m\left[\left(\frac{P}{\rho^2}\right)_{i-1}+\left(\frac{P}{\rho^2}\right)_i\right]\left(\frac{-1}{2h^2}\right) \\
&\quad -m\left[\left(\frac{P}{\rho^2}\right)_{i+1}+\left(\frac{P}{\rho^2}\right)_i\right]\left(\frac{1}{2h^2}\right)\ ,
\end{aligned}
\tag{26}
$$

since $\partial W_{ij}/\partial x_i$ is zero except for $j = i-1$ and $j = i+1$ as can be seen from Fig.3. From Eqs. 24–25 we have

$$
\frac{\partial W(x_i-x_j)}{\partial x_i} = \begin{cases} \dfrac{-1}{2h^2} & j = i-1 \\ 0 & j = i \\ \dfrac{1}{2h^2} & j = i+1\,, \end{cases}
\tag{27}
$$

which leads to Eq. 26 above. This simplifies to the central difference formula

$$
\frac{dv_i}{dt} = -\frac{1}{2h}\left[\left(\frac{P}{\rho}\right)_{i+1}-\left(\frac{P}{\rho}\right)_{i-1}\right]\ ,
\tag{28}
$$

where we have used $m/\rho = h$ for equally spaced particles.

Let us now consider the case where the boundary falls within h to the right of particle i. In this case, the $j = i+1$ term is missing but the boundary term is present. Specifically, let us assume the boundary X occurs $\sim 0.6h$ to the right of particle i where $W(x_i - X) \simeq 1/2h$. Eq. 11 then becomes

$$
\begin{aligned}
\frac{dv_i}{dt} &= -\left[\left(\frac{P}{\rho^2}\right)_X+\left(\frac{P}{\rho^2}\right)_i\right]\rho_X\left(\frac{1}{2h}\right) \\
&\quad -m\left[\left(\frac{P}{\rho^2}\right)_{i-1}+\left(\frac{P}{\rho^2}\right)_i\right]\left(-\frac{1}{2h^2}\right)\ ,
\end{aligned}
\tag{29}
$$

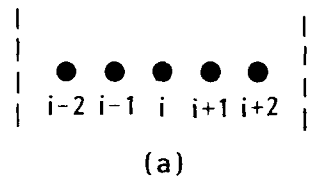

Figure 4(a). A series of equally-spaced particles far from a boundary.

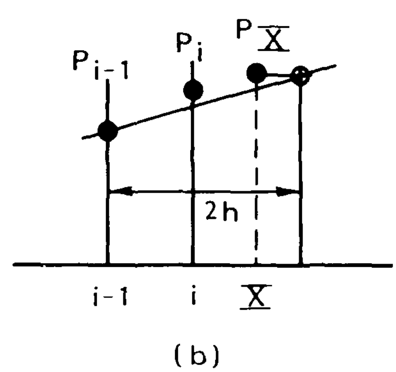

Figure 4(b). Equivalent difference form for the pressure gradient in the neighborhood of the boundary.

since $W(x_i - X) = 1/2h$ and the $j = i + 1$ term is missing. Using $h = m/\rho$, this reduces to

$$\frac{dv_i}{dt} = -\frac{1}{2h}\left[\left(\frac{P}{\rho}\right)_X - \left(\frac{P}{\rho}\right)_{i-1}\right], \tag{30}$$

which is a fairly good approximation. As shown in Fig. 4 it gives a central difference form based on P_X situated $2h$ from P_{i-1}, although it was assumed that the boundary was $\simeq 1.6h$ from x_{i-1}. All finite difference algorithms are uncertain to within $\Delta x = h$, so these boundary terms are probably as good as one would expect of most difference methods.

SECTION 5

WORK TERMS IN THE ENERGY EQUATION

We now consider the work terms which appear in the energy equation in the presence of boundary pressures. In order to insure conservation, this term must be expressed in a form that is complimentary to the right-hand side of the momentum equation so that the kinetic energy appears correctly.

We write the work terms as

$$\begin{aligned} \frac{d\epsilon}{dt} &= -\frac{P}{\rho}\frac{\partial v}{\partial x} \\ &= -\frac{\partial}{\partial x}\left(\frac{Pv}{\rho}\right) + v\frac{\partial}{\partial x}\left(\frac{P}{\rho}\right) , \end{aligned} \tag{31}$$

where ϵ is the internal energy per unit mass. Taking the kernel estimate of Eq. 31 yields

$$\begin{aligned} \frac{d\epsilon_\kappa}{dt} &= -\int_o^X \frac{\partial}{\partial x'}\left(\frac{Pv}{\rho}\right) W(x-x')dx' \\ &\quad + v_\kappa \int_o^X \frac{\partial}{\partial x'}\left(\frac{P}{\rho}\right) W(x-x')dx' , \end{aligned} \tag{32}$$

where the second term has been linearized as before. This term is now rewritten using the kernel estimate for the momentum equation,

$$\frac{dv_\kappa}{dt} = -\int_o^X \frac{\partial}{\partial x'}\left(\frac{P}{\rho}\right) W(x-x')dx' - \left(\frac{P}{\rho^2}\right)_\kappa \int_o^X \frac{\partial \rho}{\partial x'} W(x-x')dx' . \tag{33}$$

If we multiply by v_κ, we get

$$v_\kappa \int_o^X \frac{\partial}{\partial x'}\left(\frac{P}{\rho}\right) W(x-x')dx' = -v_\kappa \frac{dv_\kappa}{dt} - \left(\frac{Pv}{\rho^2}\right)_\kappa \int_o^X \frac{\partial \rho}{\partial x'} W(x-x')dx' \ , \tag{34}$$

which gives for the energy equation

$$\begin{aligned} \frac{d\epsilon_\kappa}{dt} + v_\kappa \frac{dv_\kappa}{dt} &= -\int_o^X \frac{\partial}{\partial x'}\left(\frac{Pv}{\rho}\right) W(x-x')dx' \\ &\quad - \left(\frac{Pv}{\rho^2}\right)_\kappa \int_o^X \frac{\partial \rho}{\partial x'} W(x-x')dx' \ . \end{aligned} \tag{35}$$

Next, integrating by parts we obtain

$$\begin{aligned} \frac{d\epsilon_\kappa}{dt} + v_\kappa \frac{dv_\kappa}{dt} &= -\left[\left(\frac{Pv}{\rho}\right) W\right]_o^X - \int_o^X \left(\frac{Pv}{\rho}\right) \frac{\partial W}{\partial x}(x-x')dx' \\ &\quad - \left(\frac{Pv}{\rho^2}\right)_\kappa [\rho W]_o^X - \left(\frac{Pv}{\rho^2}\right)_\kappa \int_o^X \rho \frac{\partial W}{\partial x}(x-x')dx' \ . \end{aligned} \tag{36}$$

When this expression is evaluated by the particle method, we get the energy equation expressed in terms of total energy,

$$\begin{aligned} \frac{d\epsilon_i}{dt} + \frac{d}{dt}\left(\frac{1}{2}v_i^2\right) &= \left[\left(\frac{Pv}{\rho^2}\right)_o + \left(\frac{Pv}{\rho^2}\right)_i\right] \rho_o W(x_i - o) \\ &\quad - \left[\left(\frac{Pv}{\rho^2}\right)_X + \left(\frac{Pv}{\rho^2}\right)_i\right] \rho_X W(x_i - X) \\ &\quad - \sum_j m_j \left[\left(\frac{Pv}{\rho^2}\right)_j + \left(\frac{Pv}{\rho^2}\right)_i\right] \frac{\partial W(x_i - x_j)}{\partial x_i} \ . \end{aligned} \tag{37}$$

We can verify that Eq. 37 insures conservation if we multiply by m_i and sum,

$$\begin{aligned}\frac{d}{dt}\sum_i m_i(\epsilon_i + \frac{1}{2}v_i^2) &= \frac{1}{2}(Pv)_o + \rho_o \sum_i m_i \left(\frac{Pv}{\rho}\right)_i \frac{W(x_i - o)}{\rho_i} \\ &- \frac{1}{2}(Pv)_X - \rho_X \sum_i m_i \left(\frac{Pv}{\rho}\right)_i \frac{W(x_i - X)}{\rho_i} \\ &- \sum_i \sum_j m_i m_j \left[\left(\frac{Pv}{\rho^2}\right)_j + \left(\frac{Pv}{\rho^2}\right)_i\right] \frac{\partial W(X_i - x_j)}{\partial x_i} . \end{aligned} \quad (38)$$

The left-hand side is the time rate of change of total energy, internal plus kinetic. The double sum on the right is zero because of the antisymmetry of $\partial W_{ij}/\partial x_i$. And as before, we have

$$\begin{aligned}\rho_o \sum_i m_i \left(\frac{Pv}{\rho}\right)_i \frac{W(x_i - o)}{\rho_i} &\simeq \frac{1}{2}(Pv)_o , \\ \rho_X \sum_i m_i \left(\frac{Pv}{\rho}\right)_i \frac{W(x_i - X)}{\rho_i} &\simeq \frac{1}{2}(Pv)_X , \end{aligned} \quad (39)$$

giving

$$\frac{d}{dt}\sum_i m_i(\epsilon_i + \frac{1}{2}v_i^2) = (Pv)_o - (Pv)_X . \quad (40)$$

The energy Eq. 37 is expressed in terms of the total energy. After the particles are moved using the momentum equation, the change in kinetic energy is known. Then Eq. 37 can be solved f.r the internal energy ϵ_i. In some cases, it may be desirable to have the energy equation expressed in terms of the internal energy alone.

The explicit appearance of the kinetic energy term can be eliminated using the momentum Eq. 11,

$$
\begin{aligned}
v_i \frac{dv_i}{dt} = & \left[\left(\frac{P}{\rho^2}\right)_o v_i + \left(\frac{Pv}{\rho^2}\right)_i\right] \rho_o W(x_i - o) \\
& - \left[\left(\frac{P}{\rho^2}\right)_X v_i + \left(\frac{Pv}{\rho^2}\right)_i\right] \rho_X W(x_i - X) \\
& - \sum_j m_j \left[\left(\frac{P}{\rho^2}\right)_j v_i + \left(\frac{Pv}{\rho^2}\right)_i\right] \frac{\partial W(x_i - x_j)}{\partial x_i} \ . \qquad (41)
\end{aligned}
$$

After subtraction, this leads to a form of the energy equation where the kinetic energy does not appear explicitly,

$$
\begin{aligned}
\frac{d\epsilon_i}{dt} = & [v_o - v_i] \left(\frac{P}{\rho}\right)_o W(x_i - o) \\
& - [v_X - v_i] \left(\frac{P}{\rho}\right)_X W(x_i - X) \\
& - \sum_j m_j [v_j - v_i] \left(\frac{P}{\rho^2}\right)_j \frac{\partial W(x_i - x_j)}{\partial x_i} \ . \qquad (42)
\end{aligned}
$$

In summary, we have developed a conservative expression, Eq. 37, for the work done on a fluid by pressure forces that is complementary to the momentum Eq. 11 in the presence of externally-applied (boundary) pressures. These two equations insure the conservation of momentum and energy.

SECTION 6

HEAT CONDUCTION TERMS IN THE ENERGY EQUATION

Let us now consider the addition of thermal heat conduction terms in the energy equation. This will be especially important for ICF applications. Neglecting other terms for the moment, the energy equation becomes

$$\begin{aligned} \frac{d\epsilon}{dt} &= \frac{1}{\rho}\frac{\partial}{\partial x}\left(K\frac{\partial T}{\partial x}\right) \\ &= -\frac{1}{\rho}\frac{\partial F}{\partial x} , \end{aligned} \tag{43}$$

where K is the thermal conductivity, T the temperature and F the heat flux. We shall approach this equation in the same way as the momentum equation and obtain a completely parallel formulation.

Following Section 3, we write

$$\frac{d\epsilon}{dt} = -\frac{\partial}{\partial x}\left(\frac{F}{\rho}\right) - \frac{F}{\rho^2}\frac{\partial \rho}{\partial x} , \tag{44}$$

which has the following kernel estimate

$$\begin{aligned} \frac{d\epsilon_k}{dt} = & - \int_o^X \frac{\partial}{\partial x'}\left(\frac{F}{\rho}\right) W(x - x')dx' \\ & - \left(\frac{F}{\rho^2}\right)_k \int_o^X \frac{\partial \rho}{\partial x'} W(x - x')dx' . \end{aligned} \tag{45}$$

After integration by parts, one obtains

$$
\begin{aligned}
\frac{d\epsilon_\kappa}{dt} = & - \left[\frac{F}{\rho}W(x-x')\right]_o^X - \int_o^X \left(\frac{F}{\rho}\right)\frac{\partial W}{\partial x}(x-x')dx' \\
& - \left(\frac{F}{\rho^2}\right)_k [\rho W(x-x')]_o^X \\
& - \left(\frac{F}{\rho^2}\right)_k \int_o^X \rho \frac{\partial W(x-x')}{\partial x} dx' ,
\end{aligned} \tag{46}
$$

which in particle form becomes

$$
\begin{aligned}
\frac{d\epsilon_i}{dt} = & \left[\left(\frac{F}{\rho^2}\right)_o + \left(\frac{F}{\rho^2}\right)_i\right] \rho_o W(x_i - o) \\
& - \left[\left(\frac{F}{\rho^2}\right)_X + \left(\frac{F}{\rho^2}\right)_i\right] \rho_X W(x_i - X) \\
& - \sum_j m_j \left[\left(\frac{F}{\rho^2}\right)_j + \left(\frac{F}{\rho^2}\right)_i\right] \frac{\partial W(x_i - x_j)}{\partial x_i} .
\end{aligned} \tag{47}
$$

It is clear that energy conservation follows in the same way as demonstrated above.

Thus, in Eq. 47 we have the energy equation with heat conduction in a form completely analogous to the momentum equation, Eq. 11. The boundary values for the fluxes, F_o and F_X appear in a similar way to the boundary pressures. And since experience has proven Eq. 11 to be a successful particle form of the momentum equation, one would expect similar results for Eq. 47.

There remains only to calculate the fluxes for use in Eq. 47. We write F in the form

$$
\begin{aligned}
\frac{F}{\rho} & = -K\frac{1}{\rho}\frac{\partial T}{\partial x} \\
& = -K\frac{\partial}{\partial x}\left(\frac{T}{\rho}\right) - K\frac{T}{\rho^2}\frac{\partial \rho}{\partial x} ,
\end{aligned} \tag{48}
$$

which, by a now-familiar procedure, leads to the particle equation,

$$
\begin{aligned}
\left(\frac{F}{\rho}\right)_i &= K_i \left[\left(\frac{T}{\rho^2}\right)_o + \left(\frac{T}{\rho^2}\right)_i\right] \rho_o W(x_i - o) \\
&\quad - K_i \left[\left(\frac{T}{\rho^2}\right)_X + \left(\frac{T}{\rho^2}\right)_i\right] \rho_X W(x_i - X) \\
&\quad - K_i \sum_j m_j \left[\left(\frac{T}{\rho^2}\right)_j + \left(\frac{T}{\rho^2}\right)_i\right] \frac{\partial W(x_i - x_j)}{\partial x_i} \,. \qquad (49)
\end{aligned}
$$

So the temperatures define the fluxes through Eq. 49 and the fluxes determine the energy transport through Eq. 47.

It is possible to develop an equivalent treatment of heat conduction based on the product of square root approach used in Eq. 18, but this is unlikely to be any better than the method already given. Other approaches have been proposed for heat conduction (which neglect boundary terms, however). The method of Brookshaw is discussed in the following section, and a variation of Brookshaw's method by Monaghan gives similar results in test calculations.[5]

SECTION 7

CRITIQUE OF BROOKSHAW'S METHOD OF CALCULATING THERMAL DIFFUSION

In a 1985 paper,[6] Brookshaw discusses several approaches to adding radiative heat diffusion to SPH. He describes Lucy's early attempt[7] at solving the energy equation

$$\begin{aligned} \rho T \frac{dS}{dt} &= -\frac{\partial F}{\partial x} , \\ F &= -\frac{4acT^3}{3K\rho} \frac{\partial T}{\partial x} , \end{aligned} \tag{50}$$

by using the particle method

$$\begin{aligned} \left(\rho T \frac{dS}{dt}\right)_i &= -m \sum_j \left(\frac{F}{\rho}\right)_j \frac{\partial}{\partial x_i} W(x_i - x_j) , \\ F_i &= -\left(\frac{4acT^3}{3K\rho}\right)_i m \sum_j \left(\frac{T}{\rho}\right)_j \frac{\partial W(x_i - x_j)}{\partial x_i} . \end{aligned} \tag{51}$$

It is stated that since $W(x_i - x_j) \rightarrow 0$ at the boundary of the fluid, $T \rightarrow 0$, and one has an insulating boundary condition. The statement is made, "...so there is no reason to assume that the SPH equation will automatically take into account the correct boundary condition."

It is easy to see where Lucy and Brookshaw go wrong here. In order to get the particle equations, Eq. 51, they had to integrate by parts and drop the very boundary terms they are so concerned about. For example

$$\begin{aligned} \left(\rho T \frac{dS}{dt}\right)_\kappa &= -\int_o^X \frac{\partial F}{\partial x'} W(x - x') dx' \\ &= -[FW(x - x')]_o^X - \int_o^{X'} F \frac{\partial W}{\partial x}(x - x') dx' , \end{aligned} \tag{52}$$

which becomes in particle form

$$\left(\rho T \frac{dS}{dt}\right)_i = F_o W(x_i - o) - F_X W(x_i - X) - m \sum_j \left(\frac{F}{\rho}\right)_j \frac{\partial W(x_i - x_j)}{\partial x_i} . \tag{53}$$

Even though boundary terms are present here, this is not a good form to use, since it does not guarantee conservation. It is better to use the method developed in Section 6. Test calculations showed Eq. 51 was inaccurate near the boundary and also the method was sensitive to particle positions. Brookshaw presented a different approach to calculating heat diffusion based on a difference algorithm that he claimed gives much smoother results than Eq. 51. The method given in Section 6 should be accurate near the boundaries, but it may be that Brookshaw's approach would give added smoothness. For this reason, we shall attempt to derive Brookshaw's algorithm with boundary terms included.

Write the energy equation as

$$\rho \frac{d\epsilon}{dt} = \frac{\partial}{\partial x}\left(K \frac{\partial T}{\partial x}\right) , \tag{54}$$

and form the kernel estimate

$$\rho_\kappa \frac{d\epsilon_\kappa}{dt} = \int_o^X \frac{\partial}{\partial x'} \left\{K \frac{\partial T}{\partial x}\right\} W(x - x') dx' , \tag{55}$$

where curly brackets are used to indicate a special treatment for that particular term. Integrating by parts yields

$$\rho_\kappa \frac{d\epsilon_\kappa}{dt} = \left\{K \frac{\partial T}{\partial x}\right\} W(x - x')\Big]_o^X + \int_o^X \left\{K \frac{\partial T}{\partial x'}\right\} \frac{\partial W}{\partial x}(x - x') dx' . \tag{56}$$

Now, Brookshaw appeals to a Taylor series expansion to write a difference form for the term in curly brackets.

Since

$$
\begin{aligned}
K(x') &= K(x) - (x - x')\frac{\partial K}{\partial x} + \dots \\
T(x') &= T(x) - (x - x')\frac{\partial T}{\partial x} + \frac{1}{2}(x - x')^2\frac{\partial^2 T}{\partial x^2} + \dots ,
\end{aligned} \tag{57}
$$

we can write

$$
\begin{aligned}
\left\{K\frac{\partial T}{\partial x}\right\}' &= [K(x) + K(x')]\,\frac{T(x) - T(x')}{x - x'} \\
&= 2K(x)\frac{\partial T}{\partial x} - (x - x')\left[K(x)\frac{\partial^2 T}{\partial x^2} + \frac{\partial K}{\partial x}\frac{\partial T}{\partial x}\right] + \dots
\end{aligned} \tag{58}
$$

The kernel estimate, Eq. 56, becomes

$$
\begin{aligned}
\rho_\kappa \frac{d\epsilon_\kappa}{dt} &= \left\{K\frac{\partial T}{\partial x}\right\} W(x - x')\Big]_o^X \\
&+ \int_o^X [K(x) + K(x')]\,\frac{T(x) - T(x')}{x - x'}\,\frac{\partial}{\partial x}W(x - x')dx' ,
\end{aligned} \tag{59}
$$

where Brookshaw only discusses the integral and assumes everything goes to zero at the boundaries.

It is interesting to see something like 2 $\bar{K}$ under the integral sign. To see how the difference form gives the intended heat conduction term, substitute Eq. 58 into Eq. 59

$$
\begin{aligned}
\rho_\kappa \frac{d\epsilon_\kappa}{dt} &= \left\{2K(x)\frac{\partial T}{\partial x} - (x - x')\frac{\partial}{\partial x}\left(K\frac{\partial T}{\partial x}\right) + \dots\right\} W(x - x')\Big]_o^X \\
&+ \int_o^X \left\{2K(x)\frac{\partial T}{\partial x} - (x - x')\frac{\partial}{\partial x}\left(K\frac{\partial T}{\partial x}\right) + \dots\right\}\frac{\partial}{\partial x}W(x - x')dx' .
\end{aligned} \tag{60}
$$

When the integral is performed, term-by-term cancellation gives

$$\rho_\kappa \frac{d\epsilon_\kappa}{dt} = \frac{\partial}{\partial x}\left(K\frac{\partial T}{\partial x}\right) + O(h^2) \ , \tag{61}$$

which is the result obtained by Brookshaw. Including the boundary terms in the integration by parts does not change the result given by series expansion.

Brookshaw's scheme with boundary terms can now be written as

$$\begin{aligned}\rho_\kappa \frac{d\epsilon_\kappa}{dt} &= [\{K(x) + K(x')\}\,\frac{T(x) - T(x')}{x - x'} W(x - x')]_o^X \\ &+ \int_o^X [K(x) + K(x')]\,\frac{T(x) - T(x')}{x - x'}\frac{\partial}{\partial x} W(x - x')dx' \ ,\end{aligned} \tag{62}$$

which gives in particle form

$$\begin{aligned}\frac{d\epsilon_i}{dt} &= -\frac{1}{\rho_i}\,[K_i + K_o]\,\frac{T_i - T_o}{x_i - o} W(x_i - o) + \frac{1}{\rho_i}[K_i + K_X]\frac{T_i - T_X}{x_i - X} W(x_i - X) \\ &+ m\sum_j \frac{(K_i + K_j)}{\rho_i\rho_j}\frac{T_i - T_j}{x_i - x_j}\frac{\partial}{\partial x_i} W(x_i - x_j) \ .\end{aligned} \tag{63}$$

It is clear that Eq. 63 gives conservation since the summation is antisymmetric in i and j and the necessary factors of 2 are present in the boundary terms. Whether this approach to heat conduction is better than that represented by Eqs. 47–49 can only be determined by numerical testing. Eq. 63 certainly solves the problem of an insulating boundary condition, since any particle within $2h$ of the boundary (which presumably is on the order of one diffusion length) will exchange energy with the environment represented by the temperatures T_o and T_X.

SECTION 8

CRITIQUE OF SOME MANIPULATIONS IN THE LITERATURE

In the foregoing, it has been shown that boundary terms neglected in other derivations of SPH algorithms[2-7] are essential for many problems and particularly for energy transport problems. The question arises as to how these terms were so consistently neglected over the last decade.

In Gingold and Monaghan's paper,[4] they approach the particle method as follows:

$$
\begin{aligned}
&\textit{Kernel Estimate} \quad P_\kappa(x) &&= \int P(x')W(x-x')dx' \;, \\
&\textit{Particle Approx.} \quad P_i &&= \sum_j m_j \left(\frac{P}{\rho}\right)_j W(x_i - x_j) \;, \\
&\textit{The Gradient} \quad \frac{\partial P}{\partial x_i} &&= \sum_j m_j \left(\frac{P}{\rho}\right)_j \frac{\partial W}{\partial x_i}(x_i - x_j) \;.
\end{aligned}
\tag{64}
$$

However, if one calculates the pressure gradient directly from the kernel estimate one finds:

$$
\begin{aligned}
&\textit{Kernel Estimate} \quad \left(\frac{\partial P}{\partial x}\right)_\kappa &&= \int_o^X \frac{\partial P}{\partial x'} W(x-x')dx' \;, \\
&\textit{Integration} \quad \left(\frac{\partial P}{\partial x}\right)_\kappa &&= [PW|_o^X + \int_o^X P(x')\frac{\partial W}{\partial x}(x-x')dx' \;, \\
&\textit{Particle Approx.} \quad \frac{\partial P}{\partial x_i} &&= P_X W(x_i - X) - P_o W(x_i - o) \\
& &&\quad + \sum_j m_j \left(\frac{P}{\rho}\right)_j \frac{\partial W(x_i - x_j)}{\partial x_i} \;.
\end{aligned}
\tag{65}
$$

This shows clearly that one must be careful of taking derivatives through particle approximations to kernel estimates. In Monaghan's 1982 paper,[3] he mentions integration by parts but says he is assuming W, the function, or both go to zero on the boundary. This is better than what one sees in References 4 and 6, because it is mathematically defined even though unnecessarily restrictive.

The point to be made here is that in dealing with SPH equations, it is safer to carry everything through to final form as an integral equation and only then replace the integrals with sums over particles.

SECTION 9

EXTENSION TO HIGHER DIMENSIONS

Consider first the kernel estimate for the momentum equation, Eq. 7. In vector notation, this becomes

$$\frac{d\vec{v}_\kappa}{dt} = -\int_V \nabla' \left(\frac{P}{\rho}\right) W(|\vec{r}-\vec{r}'|,h)d^3r' - \left(\frac{P}{\rho^2}\right)_\kappa \int_V \nabla'\rho W(|\vec{r}-\vec{r}'|,h)d^3r', \tag{66}$$

where we assume the kernel is spherically summetric, extending over a range R ~ 2h about the point $\vec{r}$. The volume of integration V is therefore a sphere of radius R centered on $\vec{r}$ as in Fig. 5. An exception to this is when $\vec{r}$ is within range of a boundary as in Fig. 6. Then integration by parts yields a surface term, where the boundary pressure at the surface influences the particle at point $\vec{r}$.

Integrating by parts in Eq. 66 gives

$$\frac{d\vec{v}_\kappa}{dt} = -\int_B \left(\frac{P}{\rho}\right) W(|\vec{r}-\vec{r}'|,h)d\vec{S}' - \int_V \left(\frac{P}{\rho}\right) \nabla W(|\vec{r}-\vec{r}'|,h)d^3r' - \left(\frac{P}{\rho^2}\right)_\kappa \int_B \rho W(|\vec{r}-\vec{r}'|,h)d\vec{S}' - \left(\frac{P}{\rho^2}\right)_\kappa \int_V \rho\nabla W(|\vec{r}-\vec{r}'|,h)d^3r', \tag{67}$$

where the surface integrals are over that area of the boundary intercepted by the non-zero range of W. The particle approximation to the kernel estimate becomes

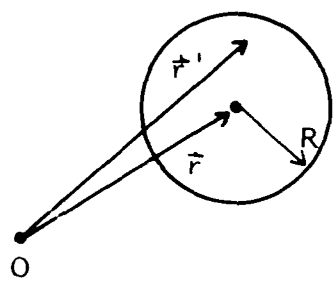

Figure 5. Range of influence of kernel $W(|\vec{r} - \vec{r}\,'|)$ about the point $\vec{r}$.

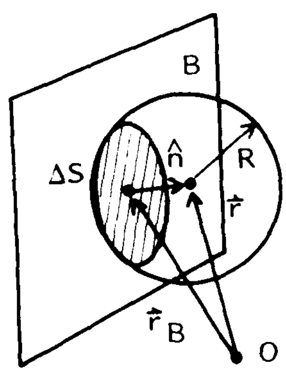

Figure 6. Range of influence of W intercepts boundary plane B over area $\Delta\vec{S}$.

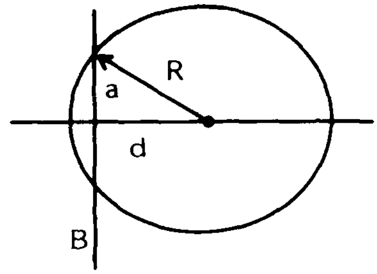

Figure 7. The area on a plane boundary intercepted by the sphere is a disk of radius a.

$$\frac{d\vec{v}_i}{dt} = -\left[\left(\frac{P}{\rho^2}\right)_B + \left(\frac{P}{\rho^2}\right)_i\right]\rho_B W(|\vec{r}_i - \vec{r}_B|, h)\Delta\vec{S}_i$$
$$-\sum_j m_j\left[\left(\frac{P}{\rho^2}\right)_j + \left(\frac{P}{\rho^2}\right)_i\right]\nabla W(|\vec{r}_i - \vec{r}_j|, h), \tag{68}$$

where ρ_B and P_B are the density and pressure at the boundary averaged over ΔS_i, $\vec{r}_B$ is the normal point at the boundary closest to $\vec{r}$, and $\hat{n}$ is the unit vector normal to the boundary at $\Delta\vec{S}_i$, all as shown in Fig. 6.

The calculation of ΔS_i is fairly easy if one neglects curvature of the boundary, which is justified in most cases since h is supposed to be small. In three dimensions, the area intercepted by a sphere of radius R located a distance $d = |\vec{r} - \vec{r}_B|$ along the normal to a plane boundary, as illustrated in Fig. 7, is

$$\Delta S_i = \pi\left(R^2 - |\vec{r} - \vec{r}_B|^2\right). \tag{69}$$

In 2D rectangular geometry (x, y) one considers a unit length in z. Hence, the range of influence of W is a cylinder of radius R and unit length. In this case, which is illustrated in Fig. 8, the area intercepted by W on a plane boundary is

$$\Delta S_i = 2\left(R^2 - |\vec{r} - \vec{r}_B|^2\right)^{1/2}. \tag{70}$$

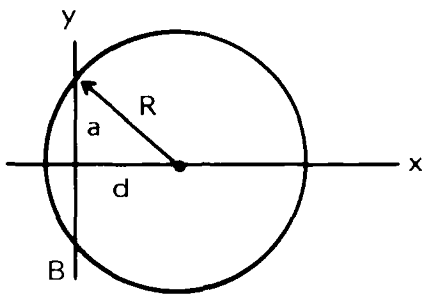

Figure 8. The area on a plane boundary intercepted by the cylinder of unit length is a rectangle of height $2a$.

This formula does not apply to the situation in 2D cylindrical geometry where, because of the symmetry, a particle is toroidal in shape. There does not appear to be a simple expression that covers all boundary configurations in this geometry. In the one-dimensional cases discussed earlier, one considers a unit length in each of the two transverse directions giving $\Delta S_i = 1$. Eq. 68 then reduces to the 1D expression derived earlier. The area ΔS_i in these three cases can be written generally as

$$\Delta S_i = C(\alpha)(R^2 - |\vec{r}_i - \vec{r}_B|^2)^{(\alpha-1)/2} , \tag{71}$$

where $\alpha = 1,2,3$ is the geometrical order, and $C(\alpha) = (1,2,\pi)$, respectively. It should be noted that an exception to Eq. 71 may occur at the corner of intersecting boundaries.

The normalization anomaly discussed in Section 2 is not altered in higher geometries. In this case, one has

$$\lim_{\vec{r}\to\vec{r}_B} \int_V W(|\vec{r} - \vec{r}'|, h) d^3r' = \frac{1}{2} , \tag{72}$$

and for a uniform distribution of particles in the neighborhood of the boundary,

$$\sum_j m_j W(|\vec{r}_B - \vec{r}_j|, h) = \frac{1}{2}\rho_c . \tag{73}$$

Likewise, the boundary value of the pressure or any similar function in the particle approximation would be expressed as

$$\frac{1}{2}P_B = \sum_j m_j \frac{P_j}{\rho_j} W(|\vec{r}_B - \vec{r}_j|, h) . \tag{74}$$

In order to demonstrate conservation of momentum from Eq. 68, one obtains the total component of momentum in any direction $\hat{x}$,

$$\begin{aligned} \sum_i m_i \frac{d\vec{v}_i}{dt} \cdot \hat{x} &= -\rho_B \sum_i m_i (P_B \Delta\vec{S}_i \cdot \hat{x}) W(|\vec{r}_i - \vec{r}_B|, h) \\ &\quad -\rho_B \sum_i m_i \left(\frac{P_i}{\rho_i^2} \Delta\vec{S}_i \cdot \hat{x} \right) W(|\vec{r}_i - \vec{r}_B|, h) , \end{aligned} \tag{75}$$

where the double sum vanishes because of the antisymmetry in i and j. The first term is the particle approximation to one-half of the boundary value of the net force on the system of particles,

$$\frac{1}{2} \sum_i (P \Delta\vec{S}_i \cdot \hat{x})_B , \tag{76}$$

and by the same arguments presented earlier in Section 3, the second term should be a good approximation to this expression also. Conservation is then expressed as

$$\sum_i m_i \frac{d\vec{v}_i}{dt} \cdot \hat{x} = \sum_i (P \Delta\vec{S}_i \cdot \hat{x})_B . \tag{77}$$

By a similar series of steps the work terms in the energy equation of Section 5 are written

$$\frac{d\epsilon_i}{dt} + \frac{d}{dt}\left(\frac{1}{2}v_i^2\right) = -\left[\left(\frac{P\vec{v}}{\rho^2}\right)_B + \left(\frac{P\vec{v}}{\rho^2}\right)_i\right] \cdot \Delta\vec{S}_i\rho_B W(|\vec{r}_i - \vec{r}_B|, h)$$
$$- \sum_j m_j \left[\left(\frac{P\vec{v}}{\rho^2}\right)_j + \left(\frac{P\vec{v}}{\rho^2}\right)_i\right] \cdot \nabla W(|\vec{r}_i - r_j|, h), \qquad (78)$$

and conservation of energy follows in a like manner,

$$\frac{d}{dt}\sum_i m_i(\epsilon_i + \frac{1}{2}v_i^2) = \sum_i (P\Delta\vec{s}_i \cdot \vec{v})_B. \qquad (79)$$

The heat flux terms in Section 6 are easily generalized to the form.

$$\frac{d\epsilon_i}{dt} = -\left[\left(\frac{\vec{F}}{\rho^2}\right)_B + \left(\frac{\vec{F}}{\rho^2}\right)_i\right] \cdot \Delta\vec{S}_i\rho_B W(|\vec{r}_i - \vec{r}_B|, h)$$
$$- \sum_j m_j \left[\left(\frac{\vec{F}}{\rho^2}\right)_j + \left(\frac{\vec{F}}{\rho^2}\right)_i\right] \cdot \nabla W(|\vec{r}_i - \vec{r}_B|, h)\ , \qquad (80)$$

with the fluxes given by

$$\left(\frac{\vec{F}}{\rho}\right)_i = -K_i\left[\left(\frac{T}{\rho^2}\right)_B + \left(\frac{T}{\rho^2}\right)_i\right] \Delta\vec{S}_i\rho_B W(|\vec{r}_i - \vec{r}_B|, h)$$
$$-K_i\sum_j m_j \left[\left(\frac{T}{\rho^2}\right)_j + \left(\frac{T}{\rho^2}\right)_i\right] \nabla W(|\vec{r}_i - \vec{r}_j|, h). \qquad (81)$$

SECTION 10

SUMMARY OF NEW SPH ALGORITHMS

A suggested approach to SPH is summarized here that allows boundary values for pressure, temperature and heat flux to be specified. This allows problems to be solved where the fluid is driven by an externally-applied pressure, temperature or both. It also allows the fluid to lose energy to a cooler environment. Although the diffusion treatment is derived for thermal conduction, radiation which is in equilibrium with the material temperature can be handled in the same way.

The momentum equation for particle i is written

$$\begin{aligned} \frac{d\vec{v}_i}{dt} &= -\left[\left(\frac{P}{\rho^2}\right)_B + \left(\frac{P}{\rho^2}\right)_i\right]\rho_B W(|\vec{r}_i - \vec{r}_B|, h)\Delta\vec{S}_i \\ &\quad - \sum_j m_j \left[\left(\frac{P}{\rho^2}\right)_j + \left(\frac{P}{\rho^2}\right)_i\right] \nabla W(|\vec{r}_i - \vec{r}_j|, h) \ . \end{aligned} \tag{82}$$

In this equation P_B is the external scalar pressure imposed on the fluid, specified as problem input. The quantity ρ_B is the boundary value of the density given by

$$\rho_B = 2\sum_j m_j W(|\vec{r}_i - \vec{r}_B|, h) \ . \tag{83}$$

The factor of 2 appears as in Eq. 74 because of the normalization anomaly at the boundary.

From Eq. 82 we see that any particle i within range of the boundary, i.e., $|\vec{r}_i - \vec{r}_B| \lesssim 2h$, begins to be influenced by the external pressure. This pressure term enters in a form similar to that of any neighboring particle except W appears in the boundary term rather than ∇W. This equation is, therefore, different than if one assumed that a fixed particle represented the boundary with a pressure defined there.

The work term which appears in the energy equation is written

$$\frac{d\epsilon_i}{dt} + \frac{d}{dt}\left(\frac{1}{2}v_i^2\right) = -\left[\left(\frac{P\vec{v}}{\rho^2}\right)_B + \left(\frac{P\vec{v}}{\rho^2}\right)_i\right] \cdot \Delta\vec{S}_i \rho_B W(|\vec{r}_i - \vec{r}_B|, h)$$
$$-\sum_j m_j \left[\left(\frac{P\vec{v}}{\rho^2}\right)_j + \left(\frac{P\vec{v}}{\rho^2}\right)_i\right] \cdot \nabla W(|\vec{r}_i - \vec{r}_j|, h). \qquad (84)$$

After the particles are moved using Eq. 82, the change in kinetic energy is known and Eq. 84 is used to obtain the change in internal energy. From the new values of ρ_i and ϵ_i, the temperatures and pressures can be calculated.

If thermal or equilibrium radiation diffusion is present, the following heat flux terms must be added to the work terms in the energy equation

$$\frac{d\epsilon_i}{dt} = Work\ Terms - \left[\left(\frac{\vec{F}}{\rho^2}\right)_B + \left(\frac{\vec{F}}{\rho^2}\right)_i\right] \cdot \Delta\vec{S}_i \rho_B W(|\vec{r}_i - \vec{r}_B|, h)$$
$$-\sum_j m_j \left[\left(\frac{\vec{F}}{\rho^2}\right)_j + \left(\frac{\vec{F}}{\rho^2}\right)_i\right] \cdot \nabla W(|\vec{r}_i - \vec{r}_j|, h). \qquad (85)$$

The heat fluxes $\vec{F}_i$ are defined at each particle position just as the pressures and temperatures are. The fluxes are obtained from the temperatures by

$$\left(\frac{\vec{F}}{\rho}\right)_j = -K_i \left[\left(\frac{T}{\rho^2}\right)_B + \left(\frac{T}{\rho^2}\right)_i\right] \Delta\vec{S}_i \rho_B W(|\vec{r}_i - \vec{r}_B|, h)$$
$$-K_i \sum_j m_j \left[\left(\frac{T}{\rho^2}\right)_j + \left(\frac{T}{\rho^2}\right)_i\right] \nabla W(|\vec{r}_i - \vec{r}_j|, h). \qquad (86)$$

It is not clear how best to implement the diffusion equation in the finite difference approximation. Some numerical experimentation may be necessary. However, the above set of SPH equations allows for boundary conditions on $P, \vec{F}$ and T and conserves energy, momentum, and mass.

SECTION 11

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